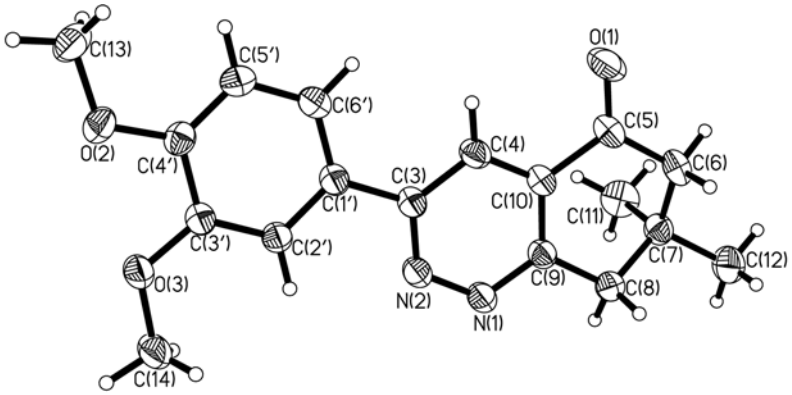
Supporting Information

A Green One-Pot Protocol for Regioselective Synthesis of New Substituted 7,8-Dihydrocinnoline-5(6*H*)-ones

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X-ray data of 3-(3,4-dimethoxyphenyl)-7,7-dimethyl-7,8-dihydrocinnolin-5(6*H*)-one (4p):



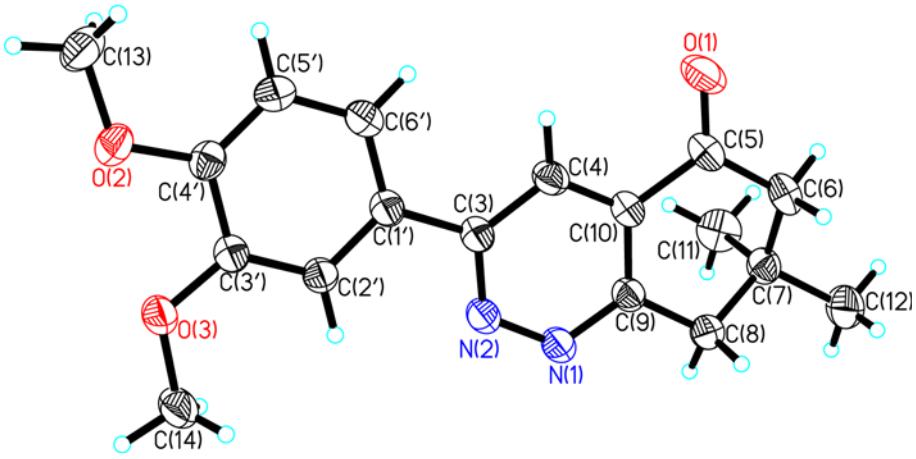


Table 1. Crystal data and structure refinement for sad1

Project path: D:\frames\JK1_E-1\work\sad1.*		
Identification code	sad1	
Empirical formula	C18 H20 N2 O3	
Formula weight	312.36	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.959(5) Å	α = 90°.
	b = 8.664(3) Å	β = 122.686(4)°.
	c = 15.815(7) Å	γ = 90°.
Volume	1609.7(11) Å^3	
Z	4	
Density (calculated)	1.289 Mg/m^3	
Absorption coefficient	0.089 mm^{-1}	
F(000)	664	
Crystal size	0.50 × 0.30 × 0.08 mm^3	
Theta range for data collection	1.73 to 28.42°.	
Index ranges	-18≤h≤18, -11≤k≤11, -21≤l≤20	
Reflections collected	19319	
Independent reflections	4019 [R(int) = 0.0347]	
Completeness to theta = 28.42°	99.4%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9930 and 0.9571	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4019 / 0 / 208	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.1262	
R indices (all data)	R1 = 0.0598, wR2 = 0.1365	
Largest diff. peak and hole	0.269 and -0.183 e.Å^{-3}	

Table 2. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for sad1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
N(1)	10217(1)	4814(1)	2914(1)	46(1)
N(2)	10873(1)	4311(1)	3864(1)	45(1)
C(3)	10422(1)	3561(1)	4308(1)	37(1)
C(4)	9254(1)	3250(2)	3785(1)	41(1)
C(5)	7326(1)	3414(2)	2199(1)	42(1)
C(6)	6655(1)	4108(2)	1171(1)	46(1)
C(7)	7318(1)	4274(2)	655(1)	42(1)
C(8)	8410(1)	5198(2)	1350(1)	45(1)
C(9)	9095(1)	4563(1)	2398(1)	37(1)
C(10)	8579(1)	3751(1)	2812(1)	36(1)
C(11)	7611(1)	2678(2)	450(1)	60(1)
C(12)	6586(1)	5151(2)	-334(1)	66(1)
O(1)	6903(1)	2613(1)	2541(1)	65(1)
C(1')	11235(1)	3093(1)	5367(1)	37(1)
C(2')	12342(1)	3708(1)	5889(1)	36(1)
C(3')	13125(1)	3294(1)	6870(1)	36(1)
C(4')	12809(1)	2253(1)	7363(1)	38(1)
C(5')	11725(1)	1642(2)	6852(1)	48(1)
C(6')	10944(1)	2062(2)	5859(1)	48(1)
O(2)	13639(1)	1954(1)	8343(1)	48(1)
C(13)	13403(1)	813(2)	8851(1)	57(1)
O(3)	14216(1)	3814(1)	7432(1)	49(1)
C(14)	14610(1)	4792(2)	6958(1)	58(1)

Table 3. Bond lengths [Å] and angles [°] for sad1

N(1)-C(9)	1.3367(16)
N(1)-N(2)	1.3415(15)
N(2)-C(3)	1.3373(15)
C(3)-C(4)	1.3995(17)
C(3)-C(1')	1.4847(17)
C(4)-C(10)	1.3698(18)
C(4)-H(4A)	0.9300
C(5)-O(1)	1.2112(16)
C(5)-C(6)	1.4956(19)
C(5)-C(10)	1.5010(17)
C(6)-C(7)	1.5361(18)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-C(11)	1.5252(19)
C(7)-C(12)	1.5302(19)
C(7)-C(8)	1.5376(17)
C(8)-C(9)	1.5004(17)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-C(10)	1.3984(17)
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(1')-C(6')	1.3824(18)
C(1')-C(2')	1.4054(17)
C(2')-C(3')	1.3776(16)
C(2')-H(2'A)	0.9300
C(3')-O(3)	1.3599(15)
C(3')-C(4')	1.4098(17)
C(4')-O(2)	1.3672(15)
C(4')-C(5')	1.3799(19)
C(5')-C(6')	1.3927(19)
C(5')-H(5'A)	0.9300
C(6')-H(6'A)	0.9300
O(2)-C(13)	1.4199(16)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
O(3)-C(14)	1.4252(16)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600

Table 3. Bond lengths [Å] and angles [°] for sad1

C(14)-H(14C)	0.9600
C(9)-N(1)-N(2)	119.83(10)
C(3)-N(2)-N(1)	121.05(10)
N(2)-C(3)-C(4)	120.76(11)
N(2)-C(3)-C(1')	115.79(10)
C(4)-C(3)-C(1')	123.45(11)
C(10)-C(4)-C(3)	118.60(11)
C(10)-C(4)-H(4A)	120.7
C(3)-C(4)-H(4A)	120.7
O(1)-C(5)-C(6)	123.08(11)
O(1)-C(5)-C(10)	120.09(12)
C(6)-C(5)-C(10)	116.83(11)
C(5)-C(6)-C(7)	114.33(10)
C(5)-C(6)-H(6A)	108.7
C(7)-C(6)-H(6A)	108.7
C(5)-C(6)-H(6B)	108.7
C(7)-C(6)-H(6B)	108.7
H(6A)-C(6)-H(6B)	107.6
C(11)-C(7)-C(12)	109.87(12)
C(11)-C(7)-C(6)	109.64(11)
C(12)-C(7)-C(6)	109.21(12)
C(11)-C(7)-C(8)	110.33(11)
C(12)-C(7)-C(8)	109.20(11)
C(6)-C(7)-C(8)	108.56(11)
C(9)-C(8)-C(7)	113.12(10)
C(9)-C(8)-H(8A)	109.0
C(7)-C(8)-H(8A)	109.0
C(9)-C(8)-H(8B)	109.0
C(7)-C(8)-H(8B)	109.0
H(8A)-C(8)-H(8B)	107.8
N(1)-C(9)-C(10)	121.72(11)
N(1)-C(9)-C(8)	116.91(11)
C(10)-C(9)-C(8)	121.36(11)
C(4)-C(10)-C(9)	118.00(11)
C(4)-C(10)-C(5)	121.30(11)
C(9)-C(10)-C(5)	120.69(11)
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(7)-C(12)-H(12A)	109.5
C(7)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(7)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(6')-C(1')-C(2')	118.62(11)
C(6')-C(1')-C(3)	122.22(11)
C(2')-C(1')-C(3)	119.16(11)
C(3')-C(2')-C(1')	120.96(11)
C(3')-C(2')-H(2'A)	119.5
C(1')-C(2')-H(2'A)	119.5
O(3)-C(3')-C(2')	125.24(11)

Table 3. Bond lengths [Å] and angles [°] for sad1

O(3)-C(3')-C(4')	115.09(10)
C(2')-C(3')-C(4')	119.67(11)
O(2)-C(4')-C(5')	125.49(11)
O(2)-C(4')-C(3')	114.96(11)
C(5')-C(4')-C(3')	119.55(11)
C(4')-C(5')-C(6')	120.22(12)
C(4')-C(5')-H(5'A)	119.9
C(6')-C(5')-H(5'A)	119.9
C(1')-C(6')-C(5')	120.97(12)
C(1')-C(6')-H(6'A)	119.5
C(5')-C(6')-H(6'A)	119.5
C(4')-O(2)-C(13)	117.39(11)
O(2)-C(13)-H(13A)	109.5
O(2)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
O(2)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(3')-O(3)-C(14)	117.84(10)
O(3)-C(14)-H(14A)	109.5
O(3)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
O(3)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for sad1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
N(1)	34(1)	60(1)	39(1)	7(1)	16(1)	-6(1)
N(2)	32(1)	60(1)	39(1)	7(1)	16(1)	-5(1)
C(3)	32(1)	42(1)	36(1)	-2(1)	18(1)	-1(1)
C(4)	35(1)	51(1)	39(1)	1(1)	22(1)	-4(1)
C(5)	32(1)	52(1)	43(1)	-8(1)	20(1)	-5(1)
C(6)	30(1)	56(1)	43(1)	-8(1)	15(1)	-1(1)
C(7)	38(1)	46(1)	35(1)	-3(1)	15(1)	-2(1)
C(8)	38(1)	46(1)	40(1)	4(1)	15(1)	-4(1)
C(9)	33(1)	38(1)	37(1)	-2(1)	17(1)	-2(1)
C(10)	30(1)	41(1)	37(1)	-4(1)	17(1)	-2(1)
C(11)	70(1)	58(1)	58(1)	-15(1)	40(1)	-4(1)
C(12)	49(1)	84(1)	43(1)	11(1)	10(1)	-6(1)
O(1)	41(1)	91(1)	61(1)	4(1)	27(1)	-18(1)
C(1')	33(1)	43(1)	35(1)	-1(1)	18(1)	0(1)
C(2')	35(1)	42(1)	34(1)	1(1)	19(1)	-1(1)
C(3')	33(1)	42(1)	33(1)	-2(1)	18(1)	0(1)
C(4')	41(1)	42(1)	35(1)	2(1)	22(1)	5(1)
C(5')	48(1)	53(1)	46(1)	8(1)	28(1)	-4(1)
C(6')	37(1)	58(1)	47(1)	4(1)	20(1)	-8(1)
O(2)	48(1)	55(1)	36(1)	10(1)	21(1)	4(1)
C(13)	64(1)	60(1)	51(1)	20(1)	34(1)	13(1)
O(3)	36(1)	69(1)	34(1)	6(1)	14(1)	-10(1)
C(14)	40(1)	87(1)	41(1)	7(1)	19(1)	-16(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for sad1

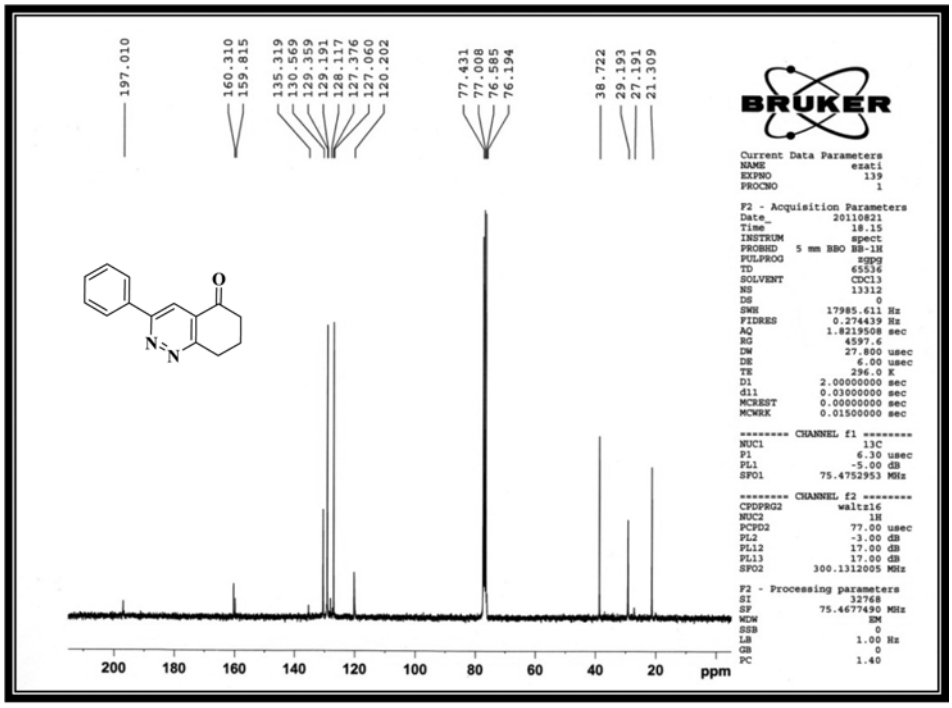
	x	y	z	U(eq)
H(4A)	8943	2714	4091	49
H(6A)	6391	5121	1219	55
H(6B)	5989	3473	752	55
H(8A)	8877	5200	1066	54
H(8B)	8208	6259	1378	54
H(11A)	6922	2115	14	89
H(11B)	8063	2131	1072	89
H(11C)	8032	2785	134	89
H(12A)	5905	4576	-772	99
H(12B)	7006	5282	-650	99
H(12C)	6390	6144	-202	99
H(2'A)	12550	4403	5567	44
H(5'A)	11514	949	7173	58
H(6'A)	10215	1641	5521	58
H(13A)	14044	715	9529	85
H(13B)	13262	-158	8511	85
H(13C)	12744	1111	8856	85
H(14A)	15388	5073	7433	86
H(14B)	14150	5707	6717	86
H(14C)	14558	4256	6403	86

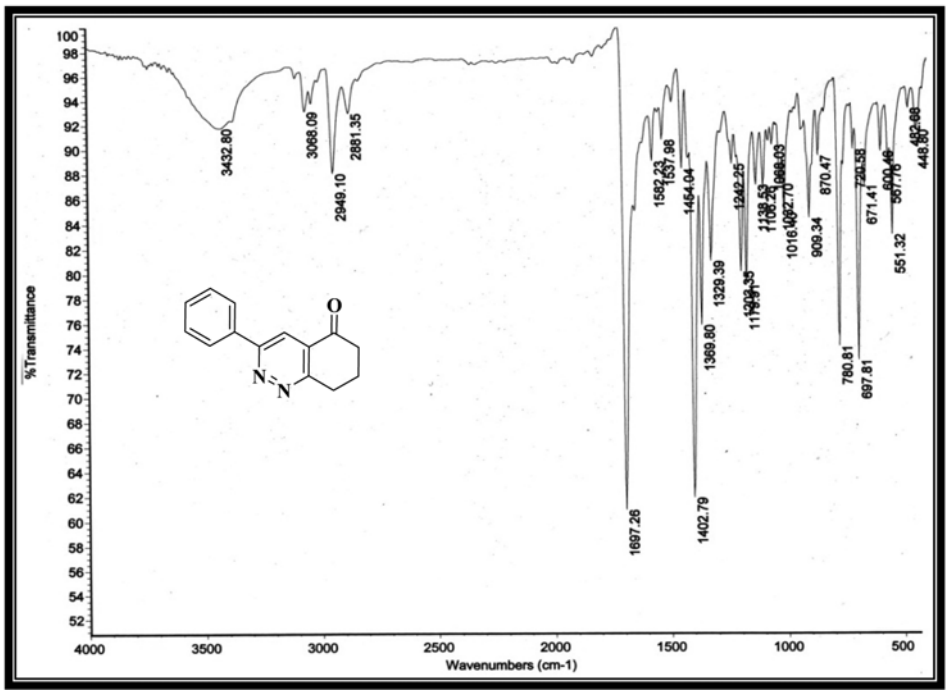
Table 6. Torsion angles [°] for sad1

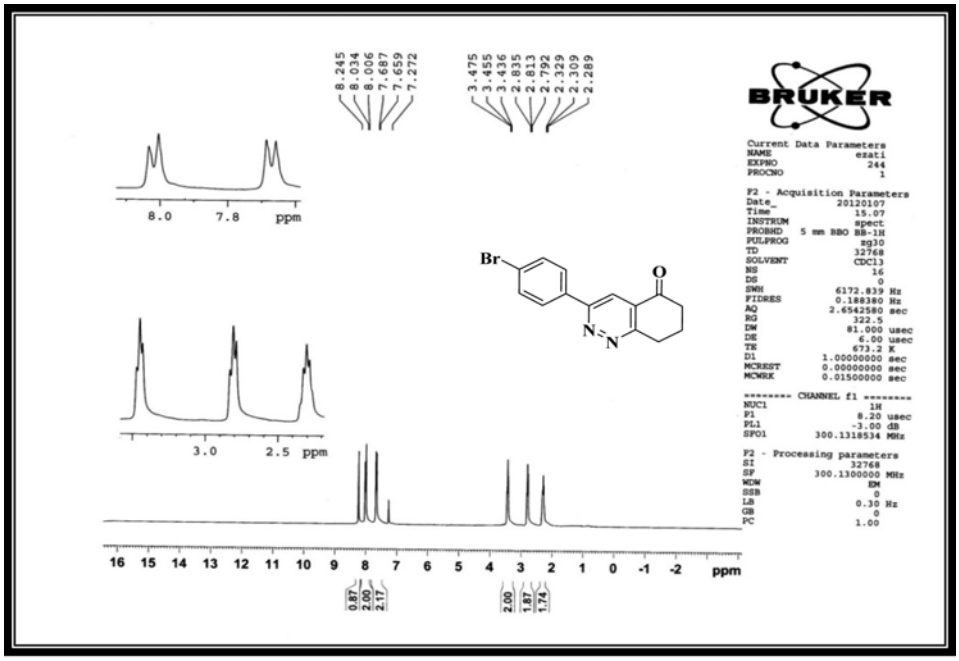
C(9)-N(1)-N(2)-C(3)	-0.15(19)
N(1)-N(2)-C(3)-C(4)	1.45(19)
N(1)-N(2)-C(3)-C(1')	-178.82(11)
N(2)-C(3)-C(4)-C(10)	-1.06(19)
C(1')-C(3)-C(4)-C(10)	179.23(11)
O(1)-C(5)-C(6)-C(7)	-147.56(13)
C(10)-C(5)-C(6)-C(7)	32.39(16)
C(5)-C(6)-C(7)-C(11)	65.62(14)
C(5)-C(6)-C(7)-C(12)	-173.95(12)
C(5)-C(6)-C(7)-C(8)	-54.98(15)
C(11)-C(7)-C(8)-C(9)	-68.36(15)
C(12)-C(7)-C(8)-C(9)	170.78(11)
C(6)-C(7)-C(8)-C(9)	51.80(15)
N(2)-N(1)-C(9)-C(10)	-1.53(19)
N(2)-N(1)-C(9)-C(8)	178.26(11)
C(7)-C(8)-C(9)-N(1)	152.36(12)
C(7)-C(8)-C(9)-C(10)	-27.85(17)
C(3)-C(4)-C(10)-C(9)	-0.54(18)
C(3)-C(4)-C(10)-C(5)	178.12(11)
N(1)-C(9)-C(10)-C(4)	1.85(19)
C(8)-C(9)-C(10)-C(4)	-177.92(11)
N(1)-C(9)-C(10)-C(5)	-176.82(11)
C(8)-C(9)-C(10)-C(5)	3.40(18)
O(1)-C(5)-C(10)-C(4)	-4.1(2)
C(6)-C(5)-C(10)-C(4)	175.89(11)
O(1)-C(5)-C(10)-C(9)	174.48(13)
C(6)-C(5)-C(10)-C(9)	-5.48(17)
N(2)-C(3)-C(1')-C(6')	-167.06(12)
C(4)-C(3)-C(1')-C(6')	12.7(2)
N(2)-C(3)-C(1')-C(2')	12.49(17)
C(4)-C(3)-C(1')-C(2')	-167.79(11)
C(6')-C(1')-C(2')-C(3')	0.03(19)
C(3)-C(1')-C(2')-C(3')	-179.53(10)
C(1')-C(2')-C(3')-O(3)	179.36(11)
C(1')-C(2')-C(3')-C(4')	-0.69(18)
O(3)-C(3')-C(4')-O(2)	1.70(16)
C(2')-C(3')-C(4')-O(2)	-178.25(10)
O(3)-C(3')-C(4')-C(5')	-179.12(11)
C(2')-C(3')-C(4')-C(5')	0.92(18)
O(2)-C(4')-C(5')-C(6')	178.58(12)
C(3')-C(4')-C(5')-C(6')	-0.5(2)
C(2')-C(1')-C(6')-C(5')	0.4(2)
C(3)-C(1')-C(6')-C(5')	179.95(12)
C(4')-C(5')-C(6')-C(1')	-0.2(2)
C(5')-C(4')-O(2)-C(13)	6.18(19)
C(3')-C(4')-O(2)-C(13)	-174.70(11)
C(2')-C(3')-O(3)-C(14)	-3.99(19)
C(4')-C(3')-O(3)-C(14)	176.05(12)

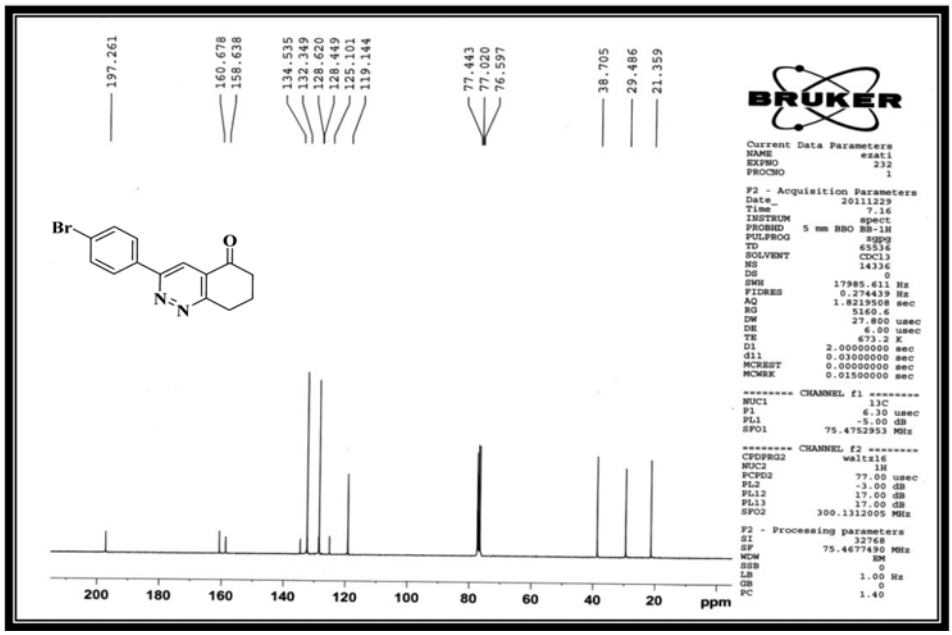
Symmetry transformations used to generate equivalent atoms:

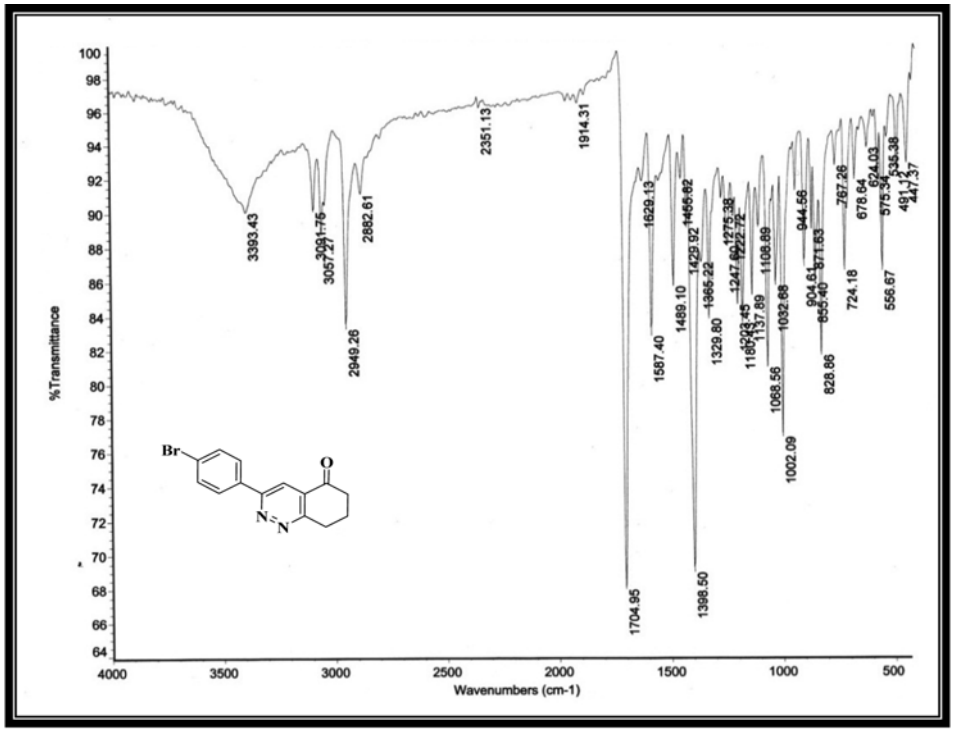
The spectra of synthesized cinnolines:

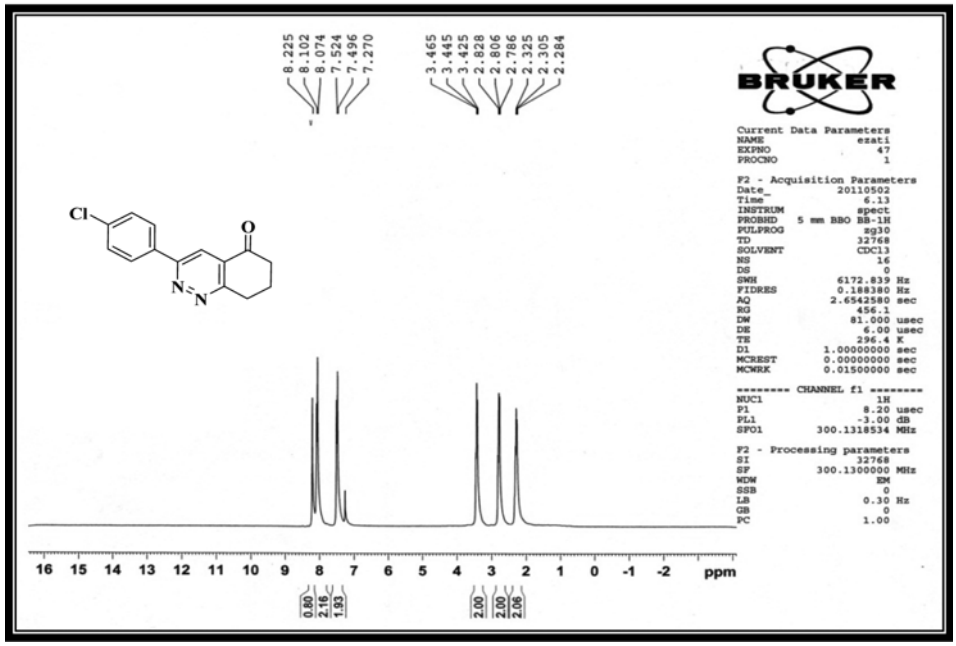


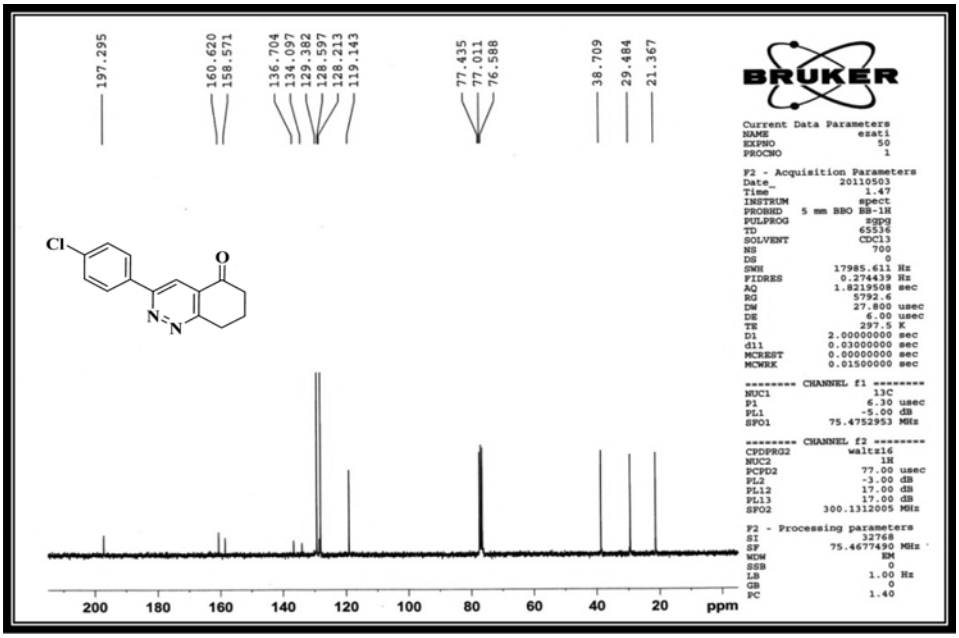


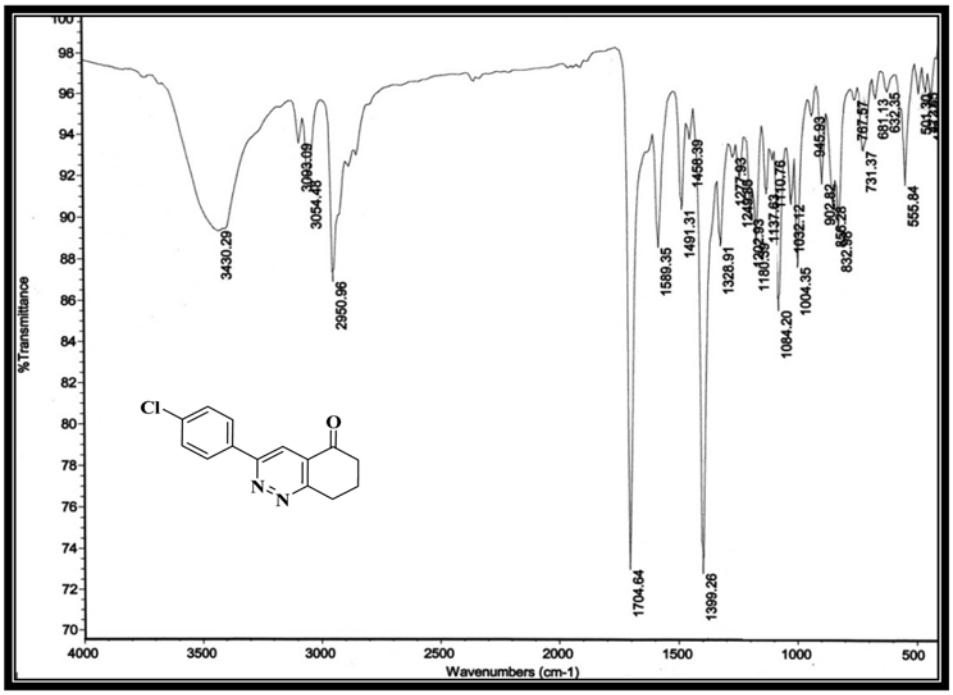

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BRUKER
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PROCNO 1
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Time 15.07
INSTRUM spect
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AQ 2.6542580 sec
RG 322.5
DW 81.000 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Br
O
N
N
8.0
7.8
ppm
3.0
2.5
ppm
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
ppm
0.87
2.00
2.17
2.00
1.87
1.74

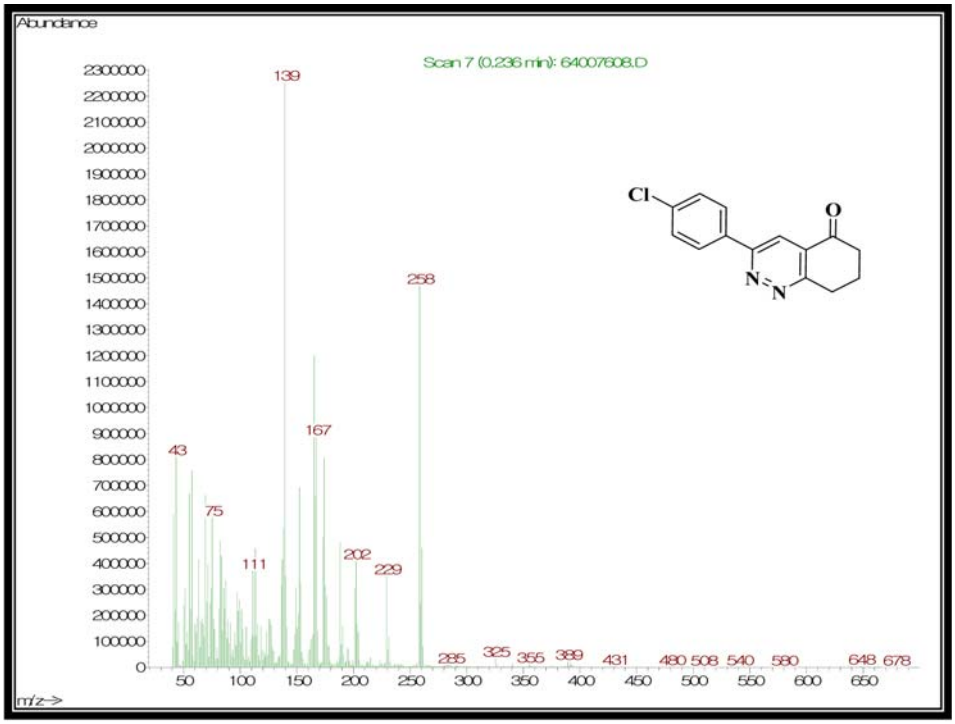

197.261
160.678
158.638
134.535
132.349
128.620
128.449
125.101
119.144
77.443
77.020
76.597
38.705
29.486
21.359
BRUKER
Current Data Parameters
NAME ezati
EXPNO 232
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111229
Time 7.16
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 14336
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 5160.6
DW 27.800 usec
DE 6.00 usec
TE 673.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.30 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 77.00 usec
PL2 -3.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Br
O
N
N
200 180 160 140 120 100 80 60 40 20
ppm

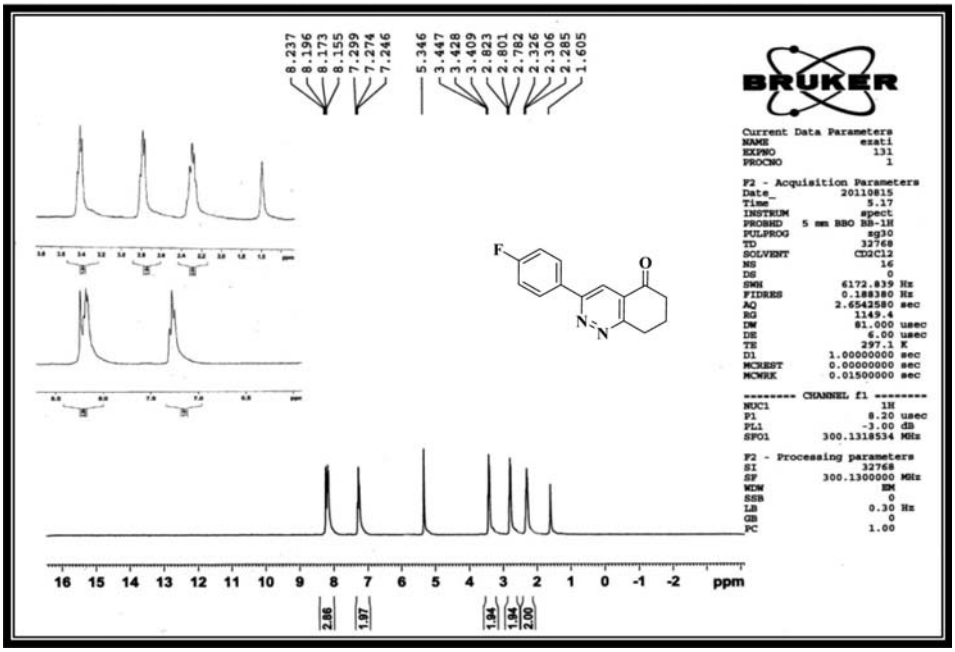

%Transmittance
Wavenumbers (cm-1)
3393.43
3091.75
3057.27
2949.26
2882.61
2351.13
1914.31
1704.95
1629.13
1587.40
1489.10
1466.62
1429.92
1398.50
1385.22
1329.80
1275.38
1247.72
1203.45
1180.43
1137.69
1108.69
1068.56
1032.68
1002.09
944.56
904.61
871.63
855.40
828.86
787.26
724.18
678.64
624.03
575.34
556.67
535.38
491.12
447.37
Br
O
N
N

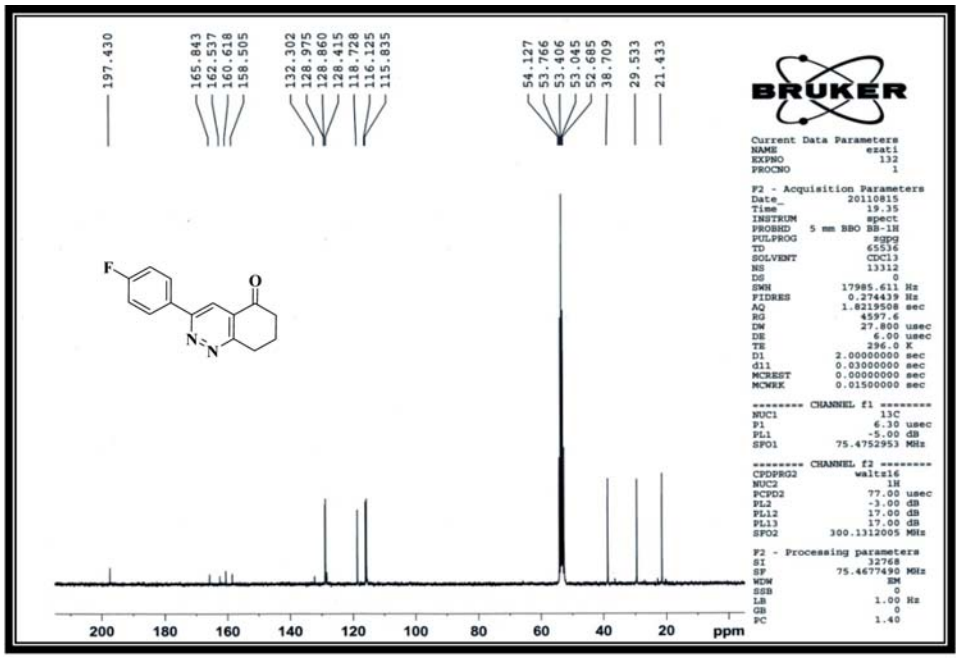

8.225
8.102
8.074
7.524
7.496
7.270
3.465
3.445
3.425
2.828
2.806
2.786
2.325
2.305
2.284
BRUKER
Current Data Parameters
NAME ezati
EXPNO 47
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110502
Time 6.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 456.1
DW 81.000 usec
DE 6.00 usec
TE 296.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.80
2.16
1.93
2.00
2.00
2.06
Cl
O
N
N

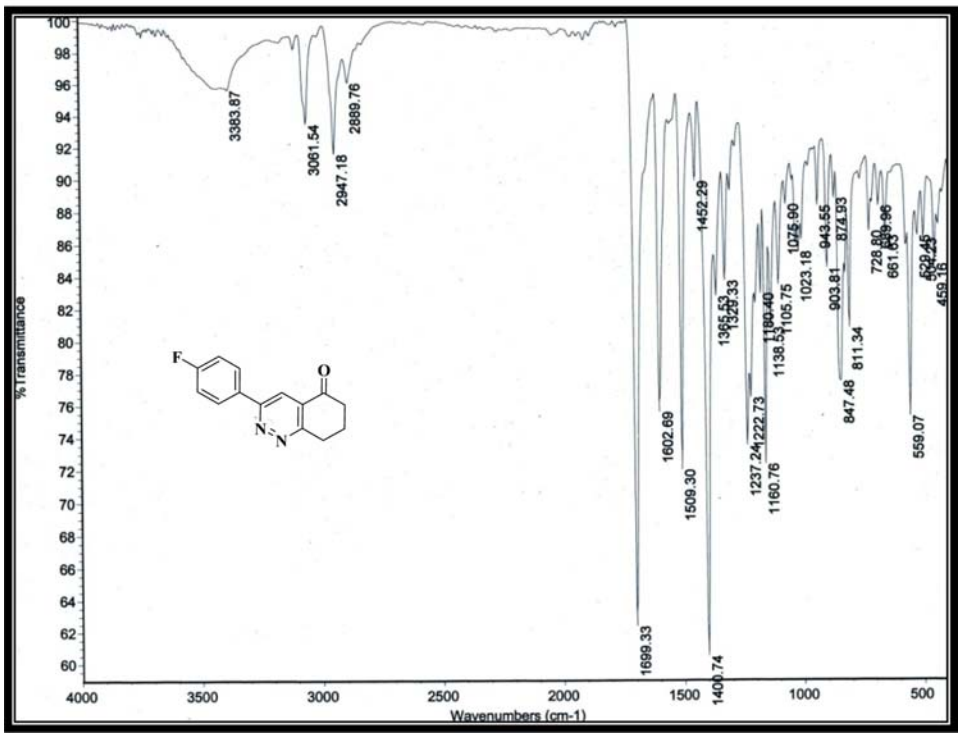

197.295
160.620
158.571
136.704
134.097
129.382
128.597
128.213
119.143
77.435
77.011
76.588
38.709
29.484
21.367
BRUKER
Current Data Parameters
NAME ezati
EXPNO 50
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110503
Time 1.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 700
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 5792.6
DW 27.800 usec
DE 6.00 usec
TE 297.5 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 6.30 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 77.00 usec
PL2 -3.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Cl
O
N
N
200
180
160
140
120
100
80
60
40
20
ppm

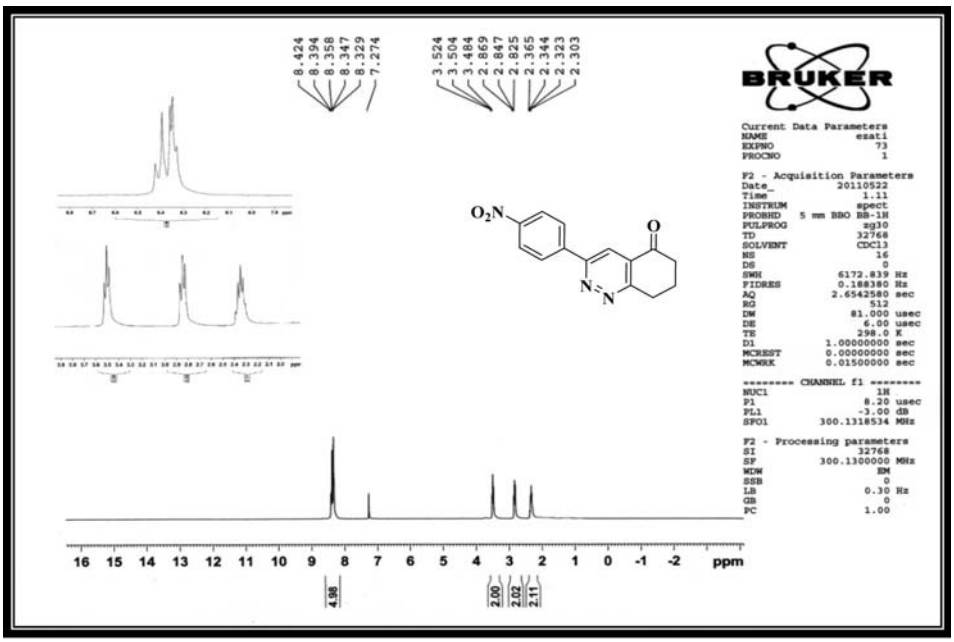

%Transmittance
3430.29
3093.09
3054.48
2950.96
1704.64
1589.35
1491.31
1458.39
1399.26
1328.91
1277.93
1180.39
1137.61
1084.20
1032.12
1004.35
945.93
902.82
832.98
731.37
681.13
632.35
555.84
Cl
O
N
N
Wavenumbers (cm-1)

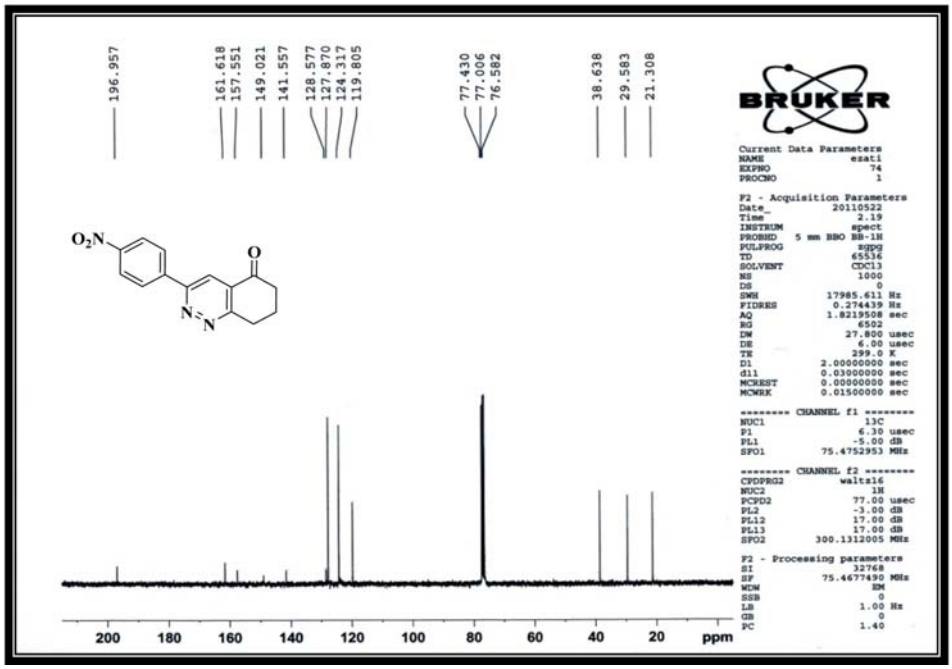

Abundance
Scan 7 (0.236 min): 64007608.D
m/z->
Cl
O
N
N
139
258
167
43
75
111
202
229
285
325
355
389
431
480
508
540
580
648
678

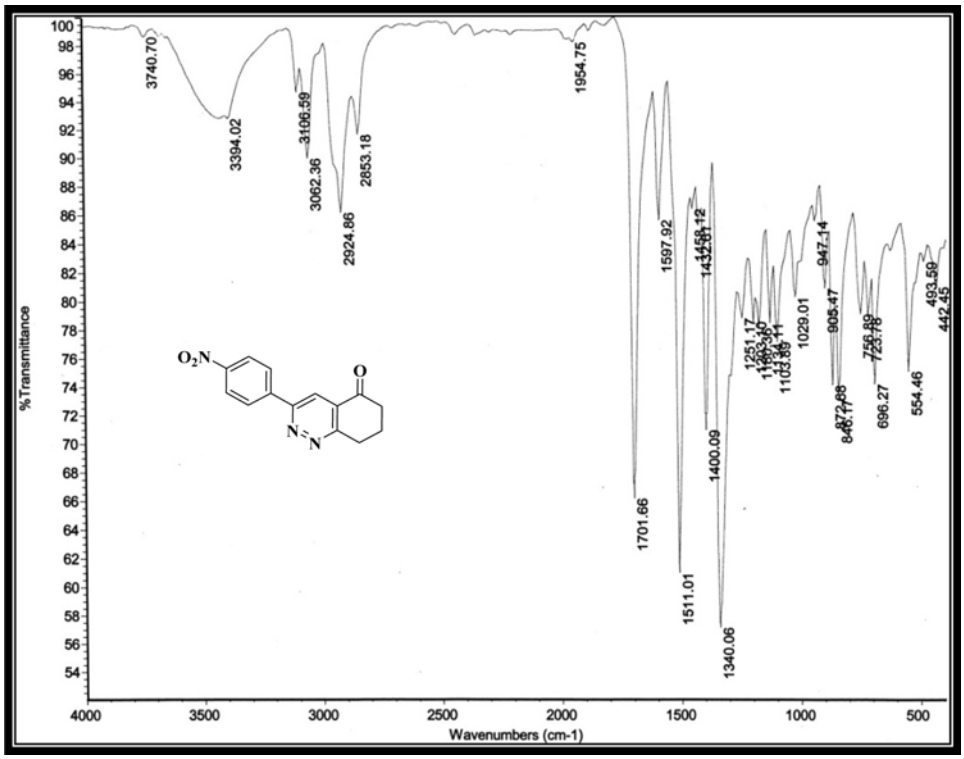

8.237
8.196
8.173
8.155
7.299
7.274
7.246
5.346
3.447
3.428
3.409
2.823
2.801
2.782
2.326
2.306
2.285
1.605
BRUKER
F
O
N
N
Current Data Parameters
NAME esati
EXPNO 131
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110815
Time 5.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CD2Cl2
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 1149.4
DW 81.000 usec
DE 6.00 usec
TE 297.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
2.86
1.97
1.94
1.84
2.00

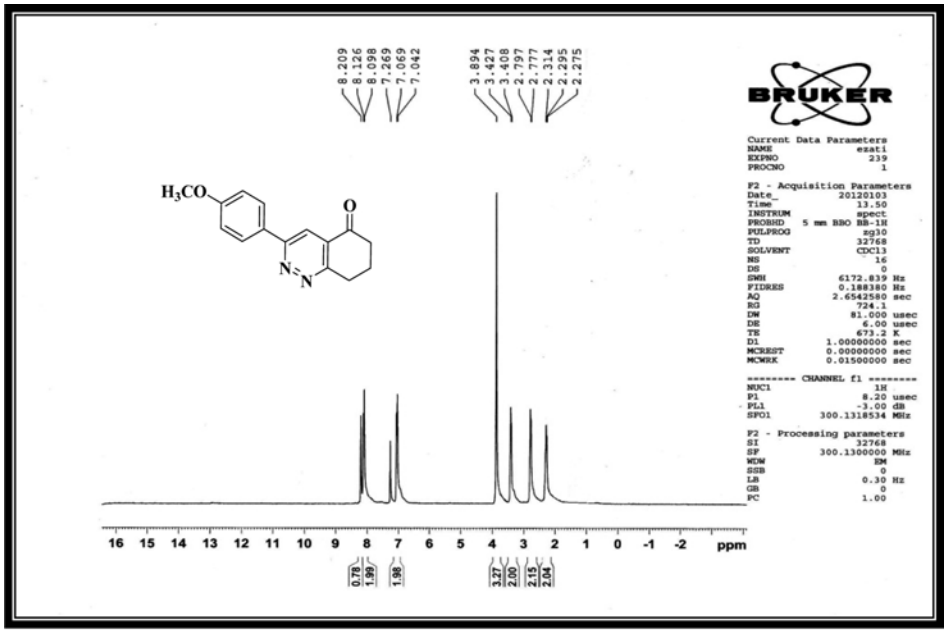

197.430
165.843
162.537
160.618
158.505
132.302
128.975
128.860
128.415
118.728
116.125
115.835
54.127
53.766
53.406
53.045
52.685
38.709
29.533
21.433
BRUKER
Current Data Parameters
NAME ezati
EXPNO 132
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110815
Time 19.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 13312
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
DW 27.800 usec
DE 6.00 usec
TE 296.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 6.30 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 77.00 usec
PL2 -3.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm

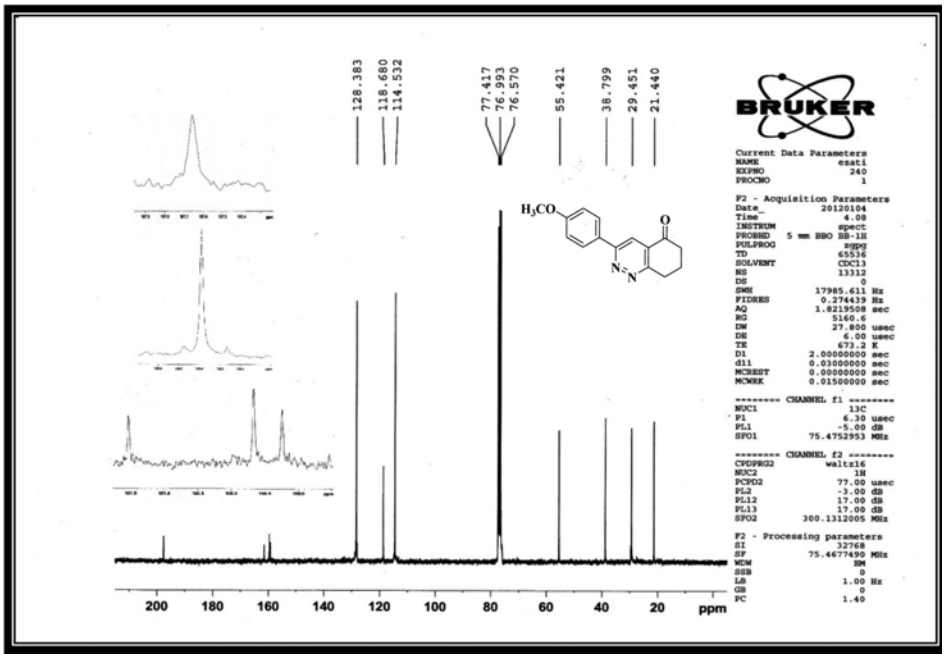

%Transmittance
3383.87
3061.54
2947.18
2889.76
1699.33
1602.69
1509.30
1452.29
1400.74
1365.53
1327.33
1237.24
1222.73
1160.76
1138.53
1105.75
1075.90
1023.18
943.55
903.81
874.93
847.48
811.34
728.80
661.03
559.07
459.16
Wavenumbers (cm-1)
4000 3500 3000 2500 2000 1500 1000 500

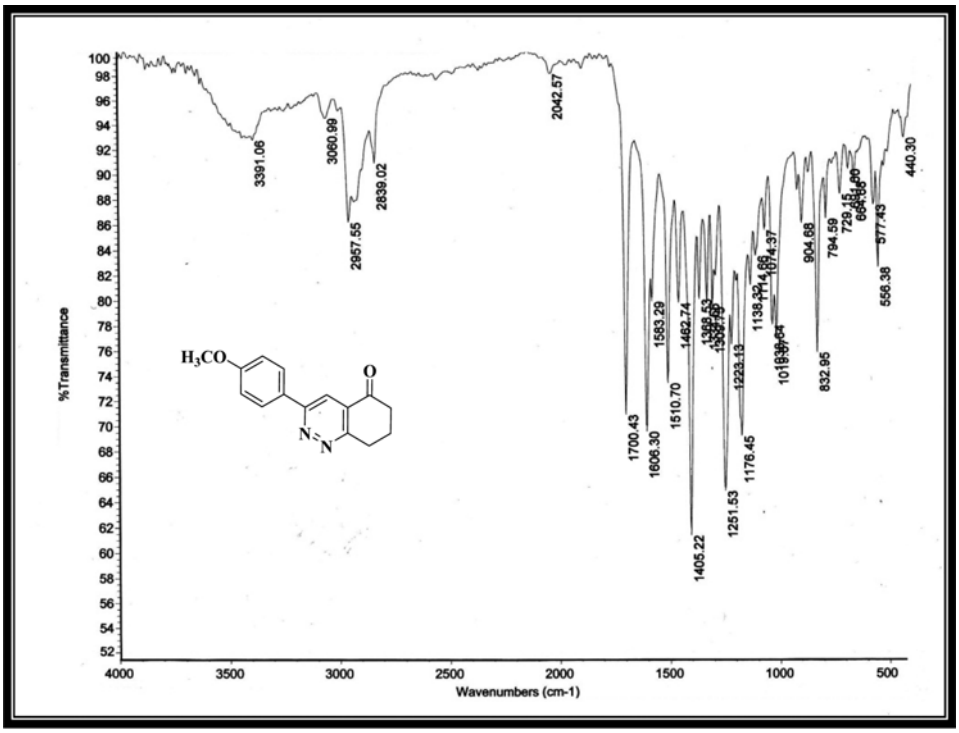

8.424
8.394
8.358
8.347
8.329
7.274
3.524
3.504
3.484
2.869
2.847
2.825
2.365
2.344
2.323
2.303
BRUKER
Current Data Parameters
NAME esati
EXPNO 73
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110522
Time_ 1.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 512
DW 81.000 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
4.98
2.00
2.02
2.11

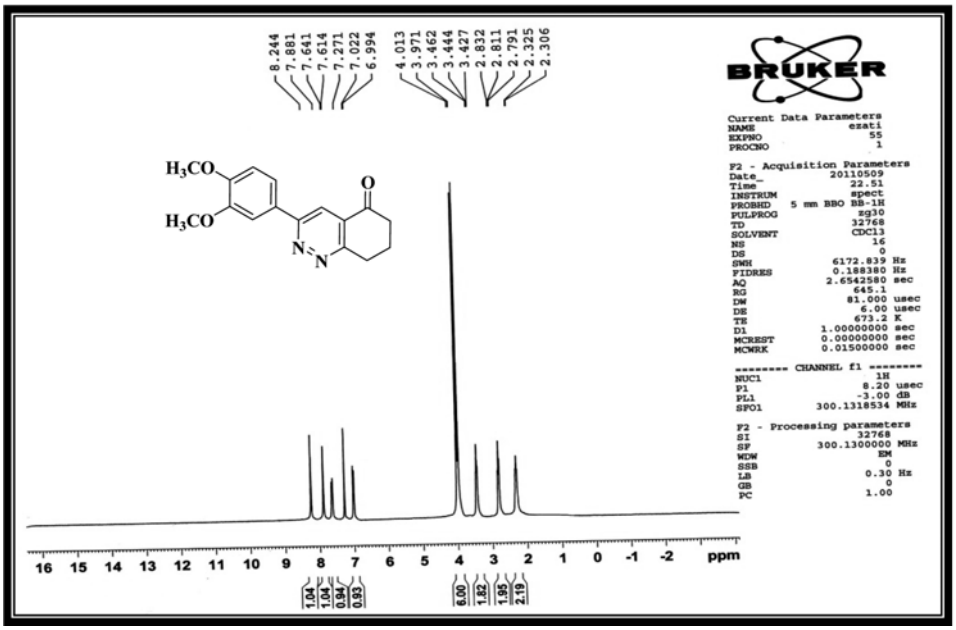

196.957
161.618
157.551
149.021
141.557
128.577
127.870
124.317
119.805
77.430
77.006
76.582
38.638
29.583
21.308
BRUKER
Current Data Parameters
NAME esati
EXPNO 74
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110522
Time_ 2.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 1000
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 6502
DW 27.800 usec
DE 6.00 usec
TE 299.0 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 6.30 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 77.00 usec
PL2 -3.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm

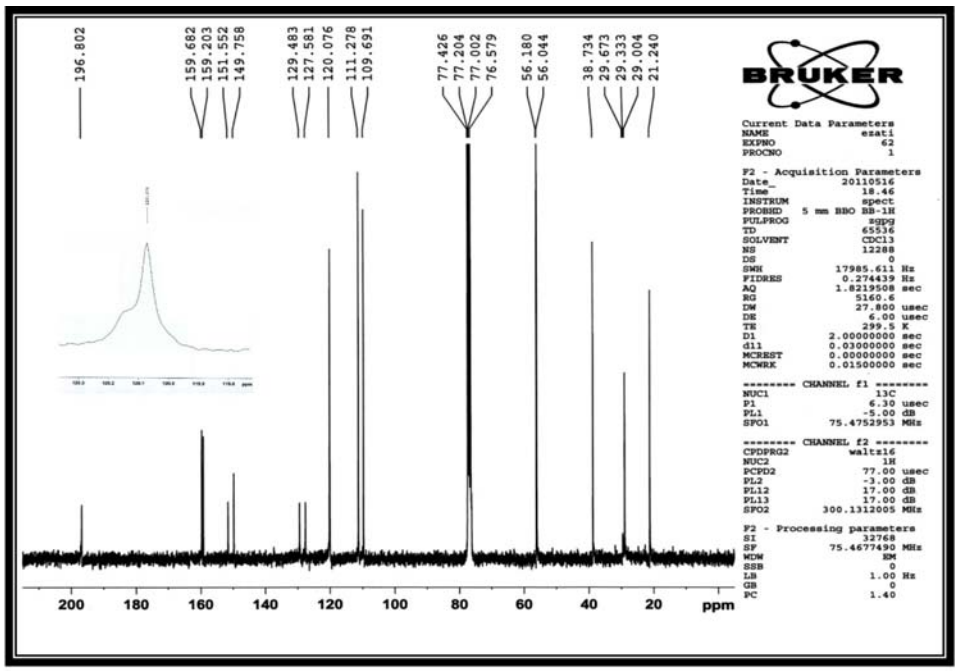

%Transmittance
Wavenumbers (cm-1)
3740.70
3394.02
3106.59
3062.36
2924.86
2853.18
1954.75
1597.92
1511.01
1400.09
1340.06
1701.66
1029.01
947.14
905.47
696.27
554.46
493.59
442.45
O2N
O
N
N

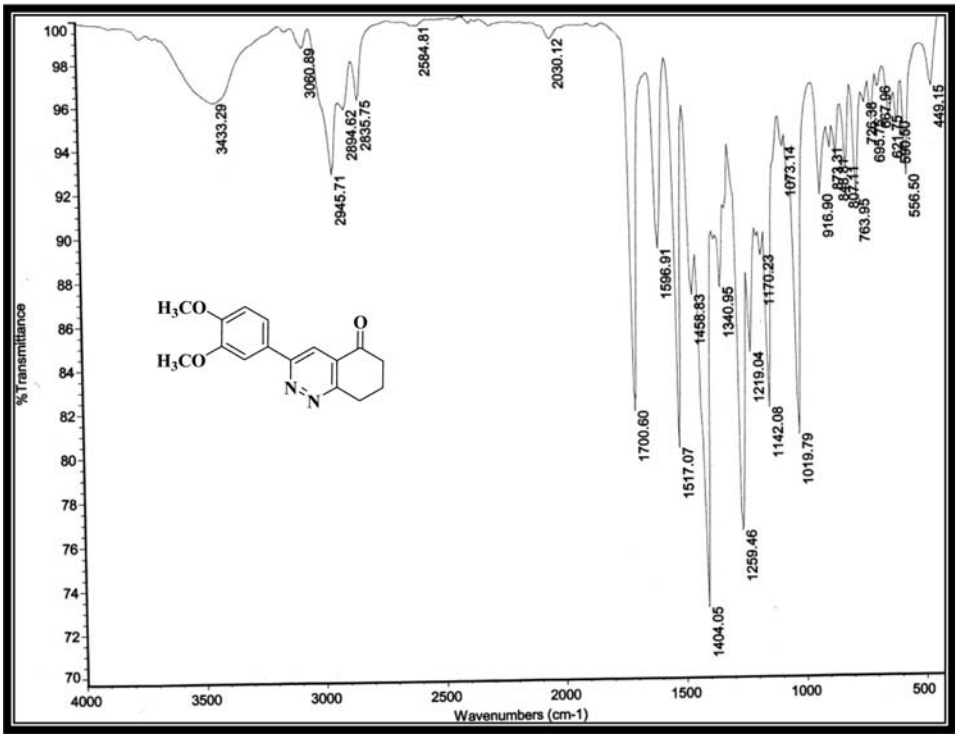

8.209
8.126
8.098
7.269
7.069
7.042
3.894
3.427
3.408
2.797
2.777
2.314
2.295
2.275
H3CO
O
N
N
BRUKER
Current Data Parameters
NAME ezat1
EXPNO 239
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120103
Time 13.50
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 724.1
DW 81.000 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.78
1.99
1.98
3.27
2.00
2.15
2.04

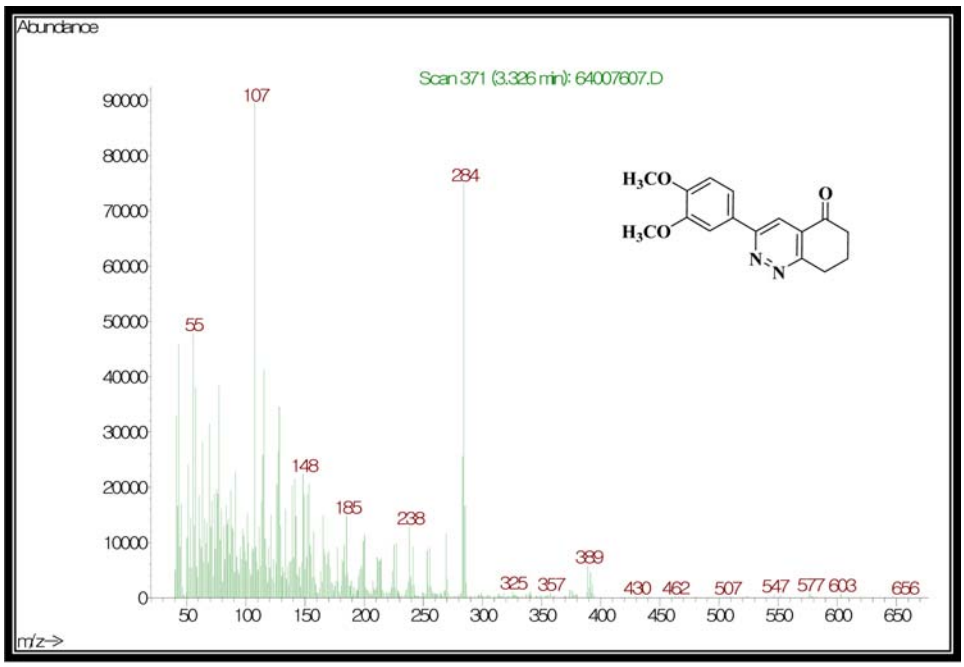

128.383
118.680
114.532
77.417
76.993
76.570
55.421
38.799
29.451
21.440
H3CO
O
N
N
BRUKER
Current Data Parameters
NAME esat1
EXPNO 240
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120104
Time 4.08
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 13312
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 5160.6
DW 27.800 usec
DE 6.00 usec
TE 673.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 6.30 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 77.00 usec
PL2 -3.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm

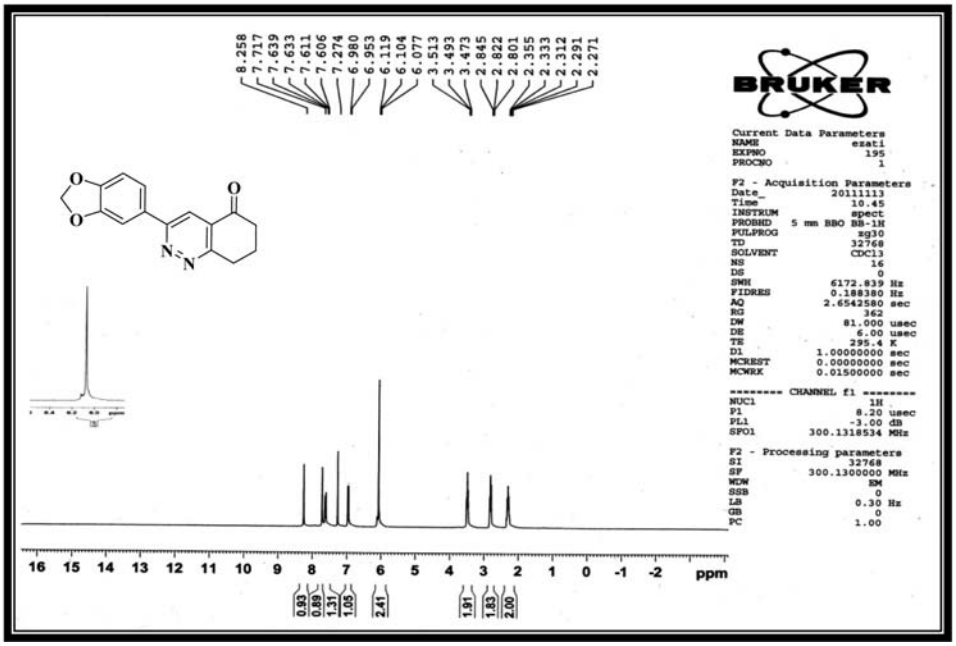

%Transmittance
Wavenumbers (cm-1)
3391.06
3060.99
2957.55
2839.02
2042.57
1700.43
1606.30
1583.29
1510.70
1462.74
1405.22
1251.53
1223.13
1176.45
1138.32
1074.37
904.68
832.95
794.59
729.15
577.43
556.38
440.30
H3CO
O
N
N

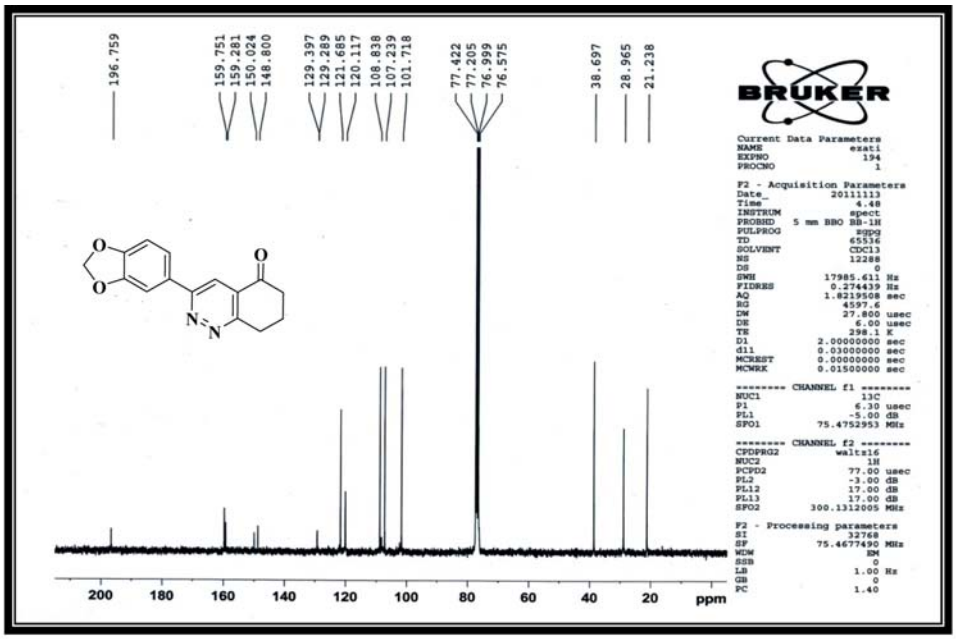

8.244
7.881
7.641
7.614
7.271
7.022
6.994
4.013
3.971
3.462
3.444
3.427
2.832
2.811
2.791
2.325
2.306
H3CO
H3CO
O
N
N
BRUKER
Current Data Parameters
NAME ezati
EXPNO 55
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110509
Time 22.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 645.1
DW 81.000 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.04
1.04
0.94
0.93
6.00
1.82
1.85
2.19

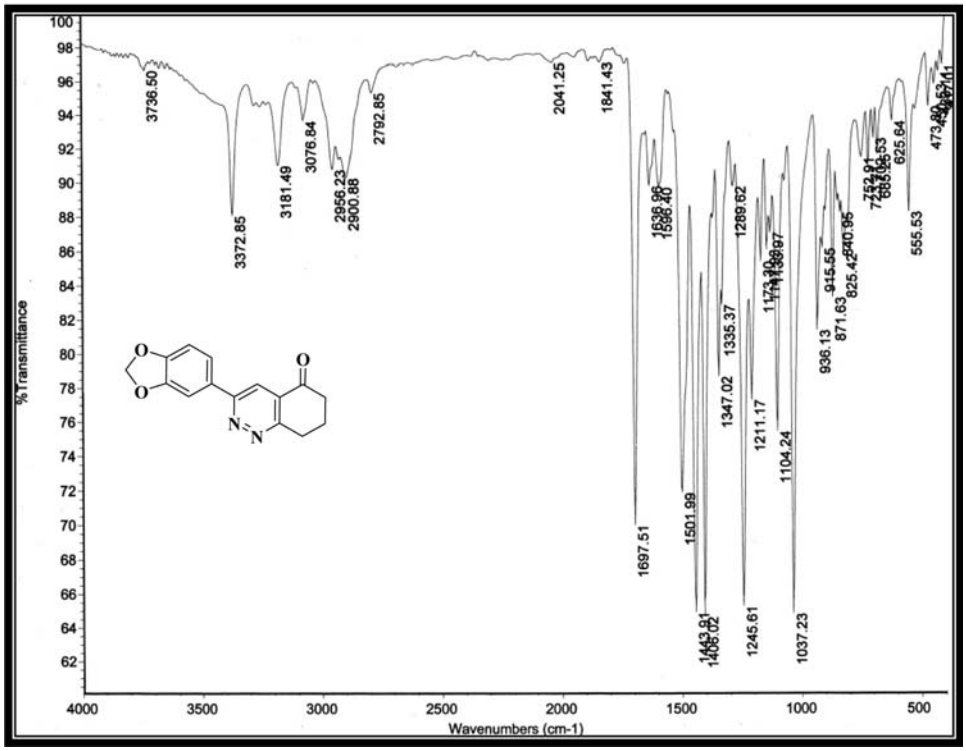

196.802
159.682
159.203
151.552
149.758
129.483
127.581
120.076
111.278
109.691
77.426
77.204
77.002
76.579
56.180
56.044
38.734
29.673
29.333
29.004
21.240
BRUKER
Current Data Parameters
NAME esati
EXPNO 62
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110516
Time 18.46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 12288
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 5160.6
DW 27.800 usec
DE 6.00 usec
TE 299.5 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 6.30 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 77.00 usec
PL2 -3.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm

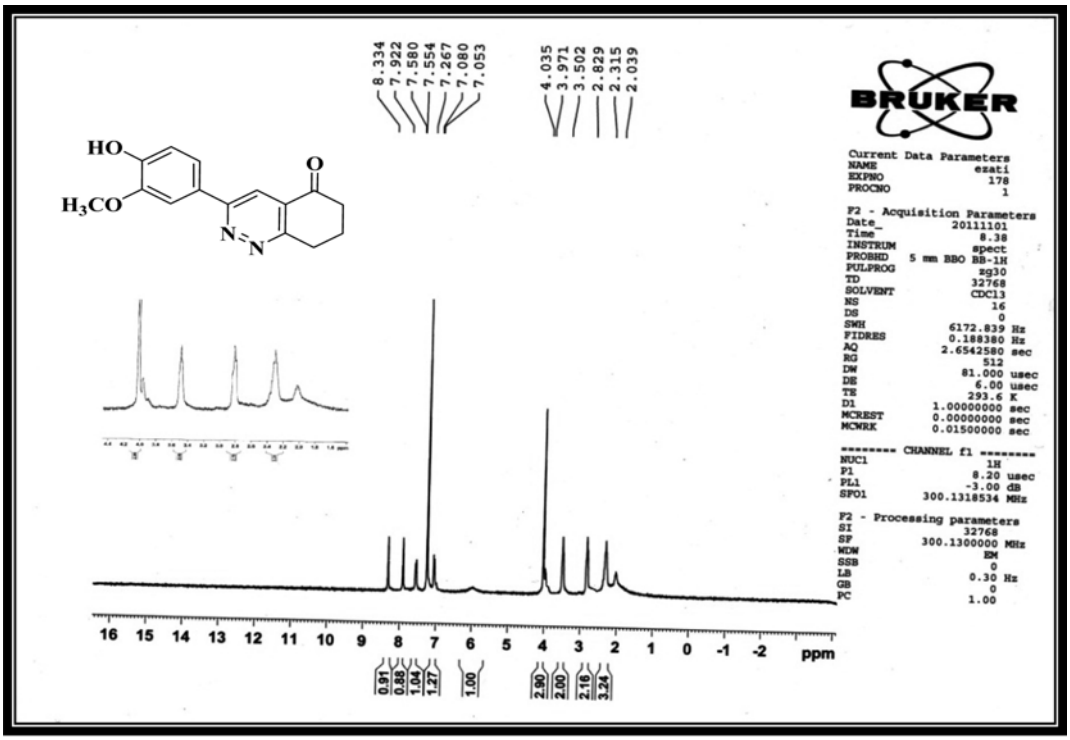

%Transmittance
Wavenumbers (cm-1)
3433.29
3060.89
2945.71
2894.62
2835.75
2584.81
2030.12
1700.60
1596.91
1517.07
1458.83
1404.05
1340.95
1259.46
1219.04
1170.23
1142.08
1073.14
1019.79
916.90
807.11
763.95
556.50
449.15
H3CO
H3CO
O
N
N


Abundance
Scan 371 (3.326 min): 64007607.D
107
284
55
148
185
238
389
325
357
430
462
507
547
577
603
656
H_3CO
H_3CO
O
N
N
m/z->


8.258
7.717
7.639
7.633
7.611
7.606
7.274
6.980
6.953
6.119
6.104
6.077
3.513
3.493
3.473
2.845
2.822
2.801
2.355
2.333
2.312
2.291
2.271
BRUKER
Current Data Parameters
NAME esati
EXPNO 195
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111113
Time 10.45
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 362
DW 81.000 usec
DE 6.00 usec
TE 295.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
N
N
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.83
0.89
1.31
1.05
2.41
1.91
1.83
2.00


196.759
159.751
159.281
150.024
148.800
129.397
129.289
121.685
120.117
108.838
107.239
101.718
77.422
77.205
76.999
76.575
38.697
28.965
21.238
BRUKER
Current Data Parameters
NAME esati
EXPNO 194
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111113
Time_ 4.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 12288
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
DW 27.800 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 13C
P1 6.30 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 77.00 usec
PL2 -3.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
ppm


%Transmittance
3736.50
3372.85
3181.49
3076.84
2956.23
2900.88
2792.85
2041.25
1841.43
1697.51
1501.99
1443.81
1408.02
1347.02
1335.37
1289.62
1245.61
1211.17
1104.24
1037.23
936.13
915.56
871.63
825.42
740.85
625.64
555.53
Wavenumbers (cm-1)


8.334
7.922
7.580
7.554
7.267
7.080
7.053
4.035
3.971
3.502
2.829
2.315
2.039
HO
H3CO
O
N
N
BRUKER
Current Data Parameters
NAME ezati
EXPNO 178
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111101
Time 8.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 512
DW 81.000 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 8.20 usec
PL1 -3.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.91
0.88
1.04
1.27
1.00
2.80
2.00
2.16
3.24